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14. ABSTRACT
Research has been performed on weighted essentially non-oscillatory schemes and discontinuous Galerkin methods, and other related numerical methods, which are high order accurate numerical methods for solving problems with shocks and other complicated solution structures. New algorithm aspects include subcell resolution for non-conservative systems, high order well balanced schemes, stable Lagrangian schemes, schemes for front propagation with obstacles, and homotopy method for steady states. Applications include high order simulations for 3D gaseous detonations, sound generation study via vortex interactions, turbulence simulations, simulations of

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Report Title

Final Report: 3.3 Numerical Analysis:High Order Accurate Algorithms for Shocks, Rapidly Changing Solutions and Multiscale Problems

ABSTRACT

Research has been performed on weighted essentially non-oscillatory schemes and discontinuous Galerkin methods, and other related numerical methods, which are high order accurate numerical methods for solving problems with shocks and other complicated solution structures. New algorithm aspects include subcell resolution for non-conservative systems, high order well balanced schemes, stable Lagrangian schemes, schemes for front propagation with obstacles, and homotopy method for steady states. Applications include high order simulations for 3D gaseous detonations, sound generation study via vortex interactions, turbulence simulations, simulations of resonant photons, and dynamic continuum models for traffic flows in urban cities with efficient and stable numerical simulations.

Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

Received		Paper
08/03/2013	1.00	Cheng Wang, Chi-Wang Shu, Wenhu Han, Jianguo Ning. High resolution WENO simulation of 3D detonation waves, Combustion and Flame, (02 2013): 0. doi: 10.1016/j.combustflame.2012.10.002
08/03/2013	5.00	Yang Yang, Ishani Roy, Chi-Wang Shu, Li-Zhi Fang. THE ANGULAR DISTRIBUTION OF Ly? RESONANT PHOTONS EMERGING FROM AN OPTICALLY THICK MEDIUM, The Astrophysical Journal, (07 2013): 0. doi: 10.1088/0004-637X/772/1/3
08/03/2013	4.00	Wenrui Hao, Jonathan D. Hauenstein, Chi-Wang Shu, Andrew J. Sommese, Zhiliang Xu, Yong-Tao Zhang. A homotopy method based on WENO schemes for solving steady state problems of hyperbolic conservation laws, Journal of Computational Physics, (10 2013): 0. doi: 10.1016/j.jcp.2013.05.008
08/03/2013	3.00	Shuhai Zhang, Hu Li, Xuliang Liu, Hanxin Zhang, Chi-Wang Shu. Classification and sound generation of two-dimensional interaction of two Taylor vortices, Physics of Fluids, (01 2013): 0. doi: 10.1063/1.4807065
08/03/2013	2.00	Olivier Bokanowski, Yingda Cheng, Chi-Wang Shu. A discontinuous Galerkin scheme for front propagation with obstacles, Numerische Mathematik, (06 2013): 0. doi: 10.1007/s00211-013-0555-3
11/13/2014	9.00	Jie Du, S.C. Wong, Chi-Wang Shu, Tao Xiong, Mengping Zhang, Keechoo Choi. Revisiting Jiang's dynamic continuum model for urban cities, Transportation Research Part B: Methodological, (10 2013): 0. doi: 10.1016/j.trb.2013.07.001
11/13/2014	10.00	Weishan Zhu, Long-long Feng, Yinhua Xia, Chi-Wang Shu, Qiusheng Gu, Li-Zhi Fang. TURBULENCE IN THE INTERGALACTIC MEDIUM: SOLENOIDAL AND DILATATIONAL MOTIONS AND THE IMPACT OF NUMERICAL VISCOSITY, The Astrophysical Journal, (11 2013): 0. doi: 10.1088/0004-637X/777/1/48
11/13/2014	11.00	Jiajia Niu, Liancun Zheng, Yang Yang, Chi-Wang Shu. Chebyshev spectral method for unsteady axisymmetric mixedconvection heat transfer of power law fluid over a cylinder withvariable transport properties, INTERNATIONAL JOURNAL OF numerical analysis and modeling, (07 2014): 525. doi:
11/13/2014	12.00	Juan Cheng, Chi-Wang Shu. Second order symmetry-preserving conservative Lagrangian scheme for compressible Euler equations in two-dimensional cylindrical coordinates, Journal of Computational Physics, (09 2014): 0. doi: 10.1016/j.jcp.2014.04.031
11/13/2014	6.00	Tao Xiong, Chi-Wang Shu, Mengping Zhang. WENO Scheme with Subcell Resolution for Computing Nonconservative Euler Equations with Applications to One-Dimensional Compressible Two-Medium Flows, Journal of Scientific Computing, (02 2012): 0. doi: 10.1007/s10915-012-9578-7
11/13/2014	7.00	Chi-Wang. Shu. On high order accurate WENO and discontinuous Galerkin schemesfor compressible turbulence simulations, Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences, (11 2012): 0. doi: 10.1098/rsta.2012.0172

11/13/2014 8.00 Yulong Xing, Chi-Wang Shu. High Order Well-Balanced WENO Scheme for the Gas Dynamics Equations Under Gravitational Fields,
Journal of Scientific Computing, (03 2012): 0. doi: 10.1007/s10915-012-9585-8

TOTAL: **12**

Number of Papers published in peer-reviewed journals:

(b) Papers published in non-peer-reviewed journals (N/A for none)

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Number of Presentations: 0.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

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Received	Paper
11/13/2014 13.00	Olivier Bokanowski, Yingda Cheng, Chi-Wang Shu. Convergence of discontinuous Galerkin schemes for frontpropagation with obstacles, Mathematics of Computation (06 2013)
TOTAL:	**1**

Number of Manuscripts:

Books

Received	Book
TOTAL:	

Received	Book Chapter
TOTAL:	

Patents Submitted

Patents Awarded

Awards

The PI, Professor Chi-Wang Shu, was elected to be a Fellow (inaugural class) of the American Mathematical Society (AMS) in November 2012.

The PI, Professor Chi-Wang Shu, was an invited 45-minute speaker in the International Congress of Mathematicians (ICM), held in Seoul, South Korea in August 2014.

Graduate Students

NAME	PERCENT_SUPPORTED	Discipline
Yang Yang	0.50	
Zheng Chen	0.20	
FTE Equivalent:	**0.70**	
Total Number:	**2**	

Names of Post Doctorates

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Names of Faculty Supported

NAME	PERCENT_SUPPORTED	National Academy Member
Chi-Wang Shu	0.10	
FTE Equivalent:	**0.10**	
Total Number:	**1**	

Names of Under Graduate students supported

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: 0.00

The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:...... 0.00

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Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):...... 0.00

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The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields:...... 0.00

Names of Personnel receiving masters degrees

NAME

Total Number:

Names of personnel receiving PHDs

NAME
Yang Yang
Zheng Chen

Total Number: **2**

Names of other research staff

NAME	PERCENT_SUPPORTED

FTE Equivalent:
Total Number:

Sub Contractors (DD882)

Inventions (DD882)

Scientific Progress

This research project is about the development, analysis, efficient implementation and application of high order accurate numerical methods for problems containing shocks, rapidly changing solutions, or multiscale problems. Weighted essentially non-oscillatory (WENO) finite difference and finite volume schemes, and discontinuous Galerkin (DG) finite element methods have been the main methods under study. Applications include computational fluid dynamics, urban traffic flow problems, and optimal control problems.

High order path-conservative schemes have been developed before in the literature for solving nonconservative hyperbolic systems. Recently, it has been observed in the literature that this approach may have some computational issues and shortcomings. We have proposed a modification to the high order path-conservative scheme to improve its computational performance and to overcome some of the shortcomings. This modification is based on the high order finite volume WENO scheme with subcell resolution and it uses an exact Riemann solver to catch the right paths at the discontinuities. An application to one-dimensional compressible two-medium flows of nonconservative or primitive Euler equations is carried out to show the effectiveness of this new approach.

The gas dynamics equations, coupled with a static gravitational field, admit the hydrostatic balance where the flux produced by the pressure is exactly canceled by the gravitational source term. Many physical problems involve the hydrodynamical evolution in a gravitational field, therefore it is essential to correctly capture the effect of gravitational force in the simulations. Improper treatment of the gravitational force can lead to a solution which either oscillates around the equilibrium, or deviates from the equilibrium after a long time run. We have designed high order well-balanced finite difference WENO schemes to this system, which can preserve the hydrostatic balance state exactly and at the same time can maintain genuine high order accuracy. Numerical tests are performed to verify high order accuracy, well-balanced property, and good resolution for smooth and discontinuous solutions. The main purpose of the well-balanced schemes designed in this work is to well resolve small perturbations of the hydrostatic balance state on coarse meshes.

The Lagrangian method and the Arbitrary Lagrangian-Eulerian method (ALE) are widely used in many fields, especially for multi-material flow simulations, due to their distinguished advantage in capturing material interfaces automatically.
We have continued on our research on the Lagrangian scheme and the remapping method, both of which constitute essential and important components of the ALE method. Specifically, we first introduce a class of high order Lagrangian schemes which are based on essentially non-oscillatory (ENO) and WENO reconstructions. The schemes are constructed both on straight-line quadrilateral meshes and on curvilinear quadrilateral meshes. Meanwhile, two approaches for high order time discretization in the Lagrangian scheme are investigated, namely, the total variation diminishing (TVD) Runge-Kutta time discretization and the Lax-Wendroff (LW) type time discretization. Next, we give a class of cell-centered Lagrangian schemes with the properties of both conservation and spherical-symmetry-preserving in two-dimensional cylindrical coordinates. After that, we summarize a high order conservative ENO remapping algorithm. Numerical experiments are shown to further demonstrate the performance of these schemes. In another work, we develop a second order cell-centered Lagrangian scheme for solving compressible Euler equations in cylindrical coordinates, based on the control volume discretizations, which is designed to have uniformly second order accuracy and capability to preserve one-dimensional spherical symmetry in a two-dimensional cylindrical geometry when computed on an equal-angle-zoned initial grid. The scheme maintains several good properties such as conservation for mass, momentum and total energy, and the geometric conservation law. Several two-dimensional numerical examples in cylindrical coordinates are presented to demonstrate the good performance of the scheme in terms of accuracy, symmetry, non-oscillation and robustness. The advantage of higher order accuracy is demonstrated in these examples.

We have developed a three-dimensional parallel solver using the fifth order high-resolution WENO finite difference scheme to perform extensive simulation for three-dimensional gaseous detonations. A careful study is conducted for the propagation modes of three-dimensional gaseous detonation wave-front structures in a long square duct. The numerical results indicate that, the instability of detonation, overdrive factor, transverse dimension and initial perturbation are the main factors that influence the appearance of spinning detonation. This study provides more insights into the mechanisms of three-dimensional gaseous detonations which would be valuable in applications.

We have investigated front propagation problems in the presence of obstacles. We propose a simple and direct DG method adapted to such front propagation problems. Our formulation leads to a level set Hamilton-Jacobi equation with constraint. The DG scheme is motivated by the variational formulation when the Hamiltonian H is a linear function of derivatives of the solution u, corresponding to linear convection problems in presence of obstacles. The scheme is then generalized to nonlinear equations, written in an explicit form. Stability analysis are performed for the linear case with Euler forward, a Heun scheme and a Runge-Kutta third order time discretization. Several numerical examples are provided to demonstrate the robustness of the method. Finally, a narrow band approach is considered in order to reduce the computational cost.
In a follow-up work we prove convergence of this DG method with the presence of singularities.

Homotopy continuation is an efficient tool for solving polynomial systems. Its efficiency relies on utilizing adaptive stepsize and adaptive precision path tracking, and endgames. We apply homotopy continuation to solve steady state problems of hyperbolic conservation laws. A third-order accurate finite difference WENO scheme with Lax-Friedrichs flux splitting is utilized to derive the difference equation. This new approach is free of the CFL condition constraint. Extensive numerical examples in both scalar and system test problems in one and two dimensions demonstrate the efficiency and robustness of the new method.

As an application in fluid dynamics, two-dimensional interaction between two Taylor vortices is simulated systematically through solving the two-dimensional, unsteady compressible Navier-Stokes equations using a fifth order WENO finite difference scheme. The main purpose of this study is to reveal the mechanism of sound generation in two-dimensional interaction of two Taylor vortices. Based on an extensive parameter study on the evolution of the vorticity field, we classify the interaction of two Taylor vortices into four types. The first type is the interaction of two counter-rotating vortices with similar strengths. The second type is the interaction of two co-rotating vortices without merging. The third type is the merging of two co-rotating vortices. The fourth type is the interaction of two vortices with a large difference in their strengths or scales. The mechanism of sound generation is analyzed.

As another application in fluid dynamics, we study the unsteady axisymmetric mixed convection boundary layer flow and heat transfer of non-Newtonian power law fluid over a cylinder. Different from most classical works, the temperature dependent variable fluid viscosity and thermal conductivity are taken into account in highly coupled velocity and temperature fields. The motion of the fluid can be modeled by a time-dependent nonlinear parabolic system in cylindrical coordinates, which is solved numerically by using Chebyshev spectral method along with the strong stability preserving (SSP) third order Runge-Kutta time discretization. We apply the numerical solver to problems with different power law indices, viscosity parameter, thermal conductivity parameter and Richardson numbers, and compute up to the steady state. The numerical solver is checked by testing the spectral convergence of the numerical approximation to a smooth exact solution of the PDEs with source terms. Moreover, the combined effects of pertinent physical parameters on the flow and heat transfer characteristics are analyzed in detail.

As an application in physics, we have investigated the angular distribution of Ly-alpha photons transferring in or emergent from an optically thick medium. Since the evolutions of specific intensity I in the frequency space and the angular space are coupled with each other, we first develop the WENO numerical solver in order to find the time-dependent solutions of the integro-differential equation of I in frequency and angular space simultaneously. We first show that the solutions with the Eddington approximation, which assume I to be linearly dependent on the angular variable mu, yield similar frequency profiles of the photon flux as that without the Eddington approximation. However, the solutions of the mu distribution evolution are significantly different from that given by Eddington approximation. First, the angular distribution of I are found to be substantially dependent on the frequency of photons. For photons with the resonant frequency nu_0, I contains only a linear term of mu. For photons with frequency at the double peaks of the flux, the mu-distribution is highly anisotropic, in which most photons are in the direction of radial forward. Moreover, either at nu_0 or at the double peaks, the mu-distributions actually are independent of the initial mu distribution of photons of the source. We also show that the optically thick medium is a collimator of photons at the double peaks. Photons from the double peaks form a forward beam with very small spread angle.

Turbulence is an important physical phenomenon, in many fluid flows. We use a suite of cosmological hydrodynamic simulations, run by two fixed grid codes, in the context of LCDM model to investigate the properties of solenoidal and dilatational, i.e, curl and compressive, motions of the intergalactic medium (IGM), and the impact of numerical viscosity on turbulence. The codes differ only in the spatial difference discretization, one is a second-order accurate total-variation-diminishing (TVD) scheme and the other is a fifth-order positivity-preserving WENO scheme. It is observed that a relatively higher numerical viscosity by the lower order TVD scheme would artificially dissipate both the compressive and vortical motions in the IGM more seriously, resulting in less developed density fluctuation and vorticity, and leading to remarkably shortened turbulence scale. This study confirms the power of high order schemes in compressible flow turbulence simulations. It also indicates the importance of guaranteed positivity-preserving property for such high speed flows.

As an application to traffic flow modeling and simulations, we study a predictive continuum dynamic user-optimal (PDUO-C) model to investigate the dynamic characteristics of traffic flow and the corresponding route-choice behavior of travelers. The modeled region is a dense urban city, which is arbitrary in shape and has a single central business district (CBD). We argue that this earlier model is not well posed due to an inconsistency in the route-choice strategy. To overcome this inconsistency, we revisit the PDUO-C problem, and construct an improved path-choice strategy. The improved model consists of a conservation law to govern the density, in which the flow direction is determined by the improved path-choice strategy, and a Hamilton-Jacobi equation to compute the total travel cost. The simultaneous satisfaction of both equations can be treated as a fixed-point problem. A self-adaptive method of successive averages (MSA) is proposed to solve this fixed-point problem. This method can automatically determine the optimal MSA step size using the least squares approach. Numerical examples are used to demonstrate the effectiveness of the model and the solution algorithm.

Technology Transfer

The algorithms that I have developed have been extensively cited and applied by scientists from government labs (e.g. NASA and DOE labs) and industry.